GISAS Data Analysis with BornAgain

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Outline

- Quick overview
- BornAgain scripting
- GUI demo
- Future plans
Overview

- April 2012: start community project for different user experiments (neutron and x-ray grazing incidence)
- Simulation and fitting of grazing incidence scattering for multilayered samples with embedded nanoparticles
- Name refers to central role of DWBA
- IsGISAXS as reference software
- More generally structured than existing software:
  - Arbitrary number of layers and/or particles
  - Polarized neutron experiments
- GUI almost in beta-release
Development history

- C++ code with Python API
- External libraries: Boost, GSL and fftw3 (+Qt for GUI)
- IsGISAXS examples as milestones along the way
- OO model facilitates extension
- Agile development
Software development: BornAgain

Programming language
- C++: speed, extensibility, maintenance
- Python API: extensibility, customization by users

Libraries
- Boost, GSL, fftw3

ROOT data analysis framework
- Standard in High Energy Physics community
- Large user base
- Scientific plotting, fitting engines, etc.

(Qt for GUI development)
Basic software architecture

User program/script

Core
Samples and algorithms

GSL

Boost

Fitting

ROOT

Graphics (only C++)

External graphics (e.g. matplotlib)
Flexible sample building

Extensible tree structure
Supported sample structures

- Multilayer
- Interface roughness
- Multiple nanoparticles (shapes, densities)
- Interference functions
- Nanoparticles assemblies
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Python API

Python script

Python wrappers

Core (C++)
Samples and algorithms
GISAS example
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Future

- GUI: beta release in September 2014
- Full support for neutron polarization
- Massive parallelization: GPU, clusters
- Input from user community and collaborations
  [http://www.bornagainproject.org](http://www.bornagainproject.org)
Thank you!